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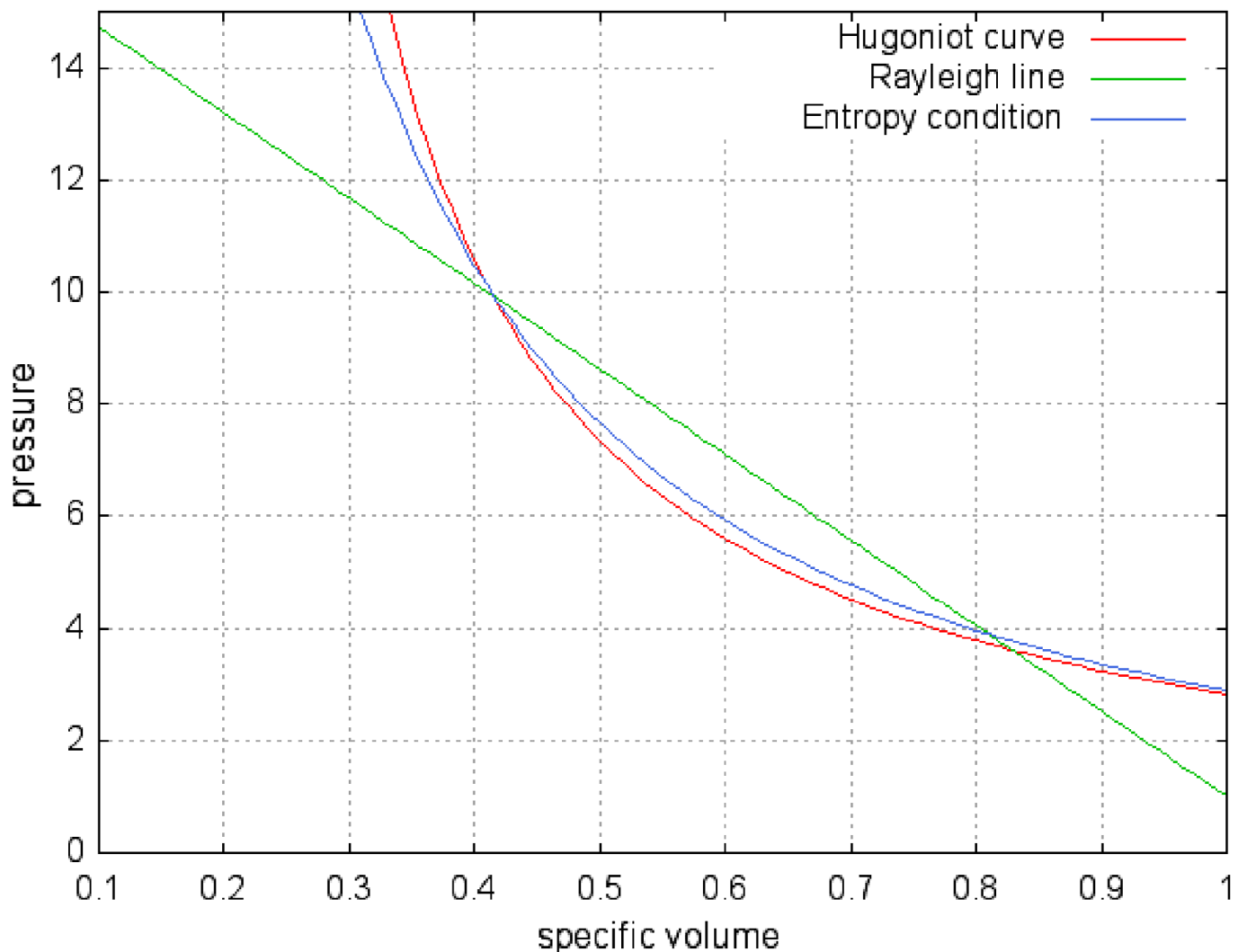
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MECHANICAL ENGINEERING | RESEARCH ARTICLE

A theory for steady and self-sustained premixed combustion waves

Weiming Liu^{1*}

Abstract: Based on the compressible Navier–Stokes equations for reactive flow problems, an eigenvalue problem for the steady and self-sustained premixed combustion wave propagation is developed. The eigenvalue problem is analytically solved and a set of analytic formulae for description of the wave propagation is found out. The analytic formulae are actually the exact solution of the eigenvalue problem in the form of integration, based on which author develops an iterative and numerical algorithm for calculation of the steady and self-sustained premixed combustion wave propagation and its speed. In order to explore the mathematical model and test the computational method developed in this paper, three groups of combustion wave propagation modes are calculated. The computational results show that the non-trivial modes of the combustion wave propagation exist and their distribution is not continuous but discrete.

Subjects: Combustion; Explosives & Blasting; Mine Safety; Reaction Engineering

Keywords: speed of combustion wave propagation; combustion velocity; fast deflagration; detonation; entropy variation of combustion wave

1. Introduction

The steady and self-sustained combustion wave plays a fundamental role in the theory of premixed combustion wave propagation. The speed of the combustion wave propagation, which is also called

ABOUT THE AUTHOR

Weiming Liu is a researcher in computational fluid dynamics (CFD). His research areas lie in three aspects, turbulence modelling, flows in complex geometries and flows with complex processes such as chemically reacting flows and phase-changing flows. His research activities are mainly to develop numerical schemes and computational algorithms to obtain high accuracy numerical solutions for the flow problems in these three areas.

PUBLIC INTEREST STATEMENT

Combustion is an important chemical reaction course. Its velocity, essentially determined by the chemical reaction rates, is one of the most important elements for us to understand, apply and control combustion processes. There have been well-developed theories for the slow combustion processes. Nonetheless, to the fast combustion processes, e.g. explosion, the theory is still incomplete. This work presents a new theoretic model that extends the classic theories into the fast combustion regimes. Under the conceptual frame of the new theory, a steady and self-sustained fast combustion wave propagation mode exists and its velocity can be obtained, which is consistent with experimental observations. Such conclusion changes our current understanding to fast combustion processes such that the fast combustion cannot be maintained by its own processes. The new theory also provides a base to develop the theory for combustion wave accelerations.

burning velocity or flame speed, is a characteristic velocity of the combustion system. Accurate determination of the wave propagation speed is therefore of great importance for the combustion theory and applications. There are two basic approaches to determine the speed of steady and self-sustained premixed combustion wave propagation. One is through solving the unsteady Navier–Stokes equations for reactive flows to obtain the wave propagation speed. In the approaches of this kind, one actually solves a Cauchy problem for the combustion wave propagation in infinitely long domain. When the numerical solution of the Cauchy problem becomes steady or fully developed, a steady and self-sustained combustion wave propagation mode is obtained. As the solution has to be developed to a steady state from a given initial state, the numerical computations often take long time. The early works of (Margolis, 1978) and (Reitz, 1981) and the recently published works (Kivotides, 2007; Pujol, Fort, Gonzalez, Montoro, & Pelegri, 2008) are the examples of numerically solving the Cauchy problem. There is also an alternative to solve the Cauchy problem, which is the asymptotics solution of the Cauchy problem (Volpert, 1997). Similar to the numerical solution of the Cauchy problem, the asymptotics solution is actually an approximate solution as well. It is also seeking for the steady combustion wave propagation modes through the wave developing from an initial state.

The second kind of approaches for determining the steady and self-sustained combustion wave propagation modes, which actually lays a foundation in today combustion theory, is directly solving an eigenvalue problem for the steady combustion wave propagations (Goldfarb, Gol'dshtein, & Kuzmenko, 1999; von Karman & Penner, 1954; Kee, Grcar, Smooke, Miller, & Meeks, 2000; Margolis & Telengator, 2001). The famous work developed in Sandia National Laboratories (Kee et al., 2000) as well as relevant computer program, PREMIX code, is solving such an eigenvalue problem for the premixed combustion wave propagation with *isobaric assumption*. The eigenvalue problem is associated with homogeneous boundary conditions. A non-trivial solution of the eigenvalue problem is called a combustion wave propagation mode. Theoretically this mode can be maintained by itself and the eigenvalue of this mode is the speed of the combustion wave propagation. In practical calculations, iterative procedures are employed to seek for the non-trivial solutions and one of the homogeneous boundary conditions is used as the criterion to judge the convergence of iteration processes. The computational practice however showed that the convergence of iterative computations is often very slow (Kee et al., 2000). The possible reason for that lacks more effective criterion for determining the convergence of solutions.

The above eigenvalue problem has yet a more serious demerit that the mathematic models for the combustion wave propagations assume that the pressure is constant during the wave propagation. In other words, the effects of pressure variation or mixture compressibility to the combustion wave propagation are neglected. This neglecting implies that the combustion waves propagate with very small wave propagation speeds, e.g. laminar flame. When the combustion waves move with fast speeds, this kind of theoretic models will not be applicable. At the moment, there are still a lot of arguments on the theory for fast, steady and self-sustained combustion waves or fast deflagrations, and the theory for fast combustion waves is still in developing stage, although they have been experimentally observed for many years, for example, see the recently published work (Wu, Burke, Son, & Yetter, 2007). Lack of the theory leads to difficultly interpret many important phenomena on fast combustion wave propagations such as deflagration-to-detonation transition (DDT) and to incorrectly understand fast combustion waves and inaccurately determine the detonation speed and so on.

The purpose of this work is to attempt to extend and improve the second kind of approaches for the steady combustion waves mentioned above. Following the second kind of approaches and based on the fully compressible Navier–Stokes equations for reactive flows, author of this paper introduces a general eigenvalue problem for the steady and self-sustained premixed combustion wave propagations with all the speeds. Analytically solving for the introduced eigenvalue problem, the author then finds out a set of exact formula for the eigenvalue, i.e. the speed of the combustion wave propagation. When iterative procedures are used to find the solutions of the introduced eigenvalue problem, the formula can be applied as the criterion to judge the convergence of numerical solutions and the scheme to update the new iteration in the iterative procedures. As the criterion and

updating scheme are based on the exact solution, the computational method developed in this work is more effective and robust over the existed approaches mentioned above. Also, the theoretic model proposed in this work covers all the combustion wave propagations such as fast deflagration and detonation, and therefore extends the range of the existed theory.

In what follows, author firstly formulates the problem and explains the differences of the model proposed in this work and existing theories. In Section 3, the raised problem is solved analytically, which results in an exact formula or mathematical relationship for the thermodynamic state after the reactions in combustions and chemical kinetics. Associated with the existed formulae, author further introduces an iterative approach for calculation of the speed of combustion wave propagation. Then, the tests of the proposed numerical method are presented in Section 4. In the numerical test section, author further discusses the nature and property of the introduced method. Finally, the conclusions are summarised up in Section 5.

2. Formulation of problems

In this paper, we study the propagation of a one-dimensional combustion wave that is sustained itself in premixed combustible gas mixture. In respect of the laboratory reference frame, the propagation course is described by the unsteady compressible Navier–Stokes equations and convection-diffusion-reaction equation for chemical species (Zeldovich, Barenblatt, Librovich, & Makhviladze, 1985):

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (1)$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) \quad (2)$$

$$\frac{\partial(\rho u E + up)}{\partial x} = -h_0^T \cdot \rho \dot{\omega} + \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \cdot u \frac{\partial u}{\partial x} + \lambda \frac{\partial T}{\partial x} \right) \quad (3)$$

$$\frac{\partial(\rho Y)}{\partial t} + \frac{\partial(\rho u Y)}{\partial x} - \frac{\partial}{\partial x} \left(\rho D \frac{\partial Y}{\partial x} \right) = \rho \dot{\omega} \quad (4)$$

Equation (1) is the continuity Equation, (2) the momentum Equation, (3) the energy Equation and (4) the chemical reaction equations. In the equations, u , ρ , p , T , E , Y , h_0 and $\dot{\omega}$ denote the flow velocity, density, pressure, temperature, total energy, vector of mass fraction of reactants, vector of heats of combustion (enthalpy of formation) and vector of reactant production rates, respectively, in which $\sum Y_i = 1$ and $\sum \omega_i = 0$, and μ , λ and D denote the mixture viscosity, conductivity and tensor of mass diffusivity, respectively. The vector of reactant production rates is controlled by the detailed chemical kinetics (Williams, 1985). The dimension for the vector of mass fraction of reactants, the vector of heats of combustions, the vector of reactant production rates and the tensor of mass diffusivity is equal to the number of species of reactants.

In order to solve the speed of the combustion wave we re-formulate (1)–(3). After reformulating, one can more clearly see the mathematic properties and physical implication the Equations (1)–(4) have. The reformulation also enables us to construct a solvable eigenvalue problem and therefore plays an importantly role in the whole work. The detailed mathematic derivations for the following contexts are given in Appendix A of this paper.

2.1. Entropy equation

Applying the transformation of hyperbolical system (5) (Courant & Friedrichs, 1976), one can rewrite the Equations (1)–(3) into (6)–(8)

$$\frac{\partial \vec{v}}{\partial \vec{w}} = \left(\frac{\partial \vec{w}}{\partial \vec{v}} \right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{u}{\rho} & \frac{1}{\rho} & 0 \\ \frac{(\gamma-1)u^2}{2} & -(\gamma-1)u & \gamma-1 \end{pmatrix} \quad (5)$$

$$\text{where } \vec{w} = (\rho \quad \rho u \quad \rho E)^T \text{ and } \vec{v} = (\rho \quad u \quad p)^T.$$

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial(u)}{\partial x} = 0 \quad (6)$$

$$\frac{\partial(u)}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial(p)}{\partial x} = \frac{1}{\rho} \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) \quad (7)$$

$$\frac{\partial(p)}{\partial t} + \gamma p \frac{\partial u}{\partial x} + u \frac{\partial(p)}{\partial x} = (\gamma-1) \left[-\rho \dot{w} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right] \quad (8)$$

The system of Equations (6)–(8) has three Riemann invariants which are written in (9)

$$(R_1 \quad R_2 \quad R_3)^T \equiv \left(\frac{p}{\rho^\gamma} \quad u - \frac{2a}{\gamma-1} \quad u + \frac{2a}{\gamma-1} \right)^T \quad (9)$$

The equation the first Riemann invariant satisfies can be written as (10). The detailed derivation of (10) is seen in Appendix A.

$$\begin{aligned} \frac{\partial \ln R_1}{\partial t} + u \frac{\partial \ln R_1}{\partial x} &= -\gamma \frac{(\gamma-1) \left[-\rho \dot{w} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{a^2} \\ &= -\frac{(\gamma-1) \left[-\rho \dot{w} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} \end{aligned} \quad (10)$$

where R_1 denotes the first Riemann invariant defined in (9). Considering the continuity Equation (1), the Equation (10) is rewritten as the conservative form:

$$\frac{\partial(\rho \ln R_1)}{\partial t} + \frac{\partial(\rho u \ln R_1)}{\partial x} = -\frac{(\gamma-1) \left[-\rho \dot{w} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} \quad (11)$$

Equation (10) represents the variation of the Riemann invariant through the chemical reaction zone of the combustion wave. It is seen that if there are no chemical reactions, the right-hand side terms of (10) or (11) will disappear and the flow becomes isentropic and the Riemann invariant keeps constant. However, when the chemical reactions exist, they work as the sources or forces to drive the wave movement, which results in the increase in the entropy of the mixture. In the following section, based on Equation (11), an eigenvalue problem is introduced for the propagation of steady combustion waves.

2.2. Eigenvalue problem

A combustion wave in the ignition and growth stages is unsteady. If the ambient condition is homogeneous, the wave will approach from the growth stage or unsteady state to a steady state that is sustained itself finally. When the steady state is reached, the combustion wave will have a constant group speed. This constant group speed is just the speed of the combustion wave propagation. If a Galilean transformation with the wave speed is applied to the unsteady Equations (1)–(4), the equations will become steady in the form which are written as follows.

$$\frac{\partial(\rho u)}{\partial x} = 0 \quad (12)$$

$$\frac{\partial}{\partial x} \left[\rho u^2 + p - \eta \frac{\partial u}{\partial x} \right] = 0 \quad (13)$$

$$\frac{\partial(\rho u E + up)}{\partial x} = -h_0^T \cdot \rho \dot{\omega} + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \quad (14)$$

$$\frac{\partial}{\partial x} \left(\rho u Y - \rho D \frac{\partial Y}{\partial x} \right) = \rho \dot{\omega} \quad (15)$$

$$\frac{\partial(\rho u \ln R_1)}{\partial x} = - \frac{(\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} \quad (16)$$

where (12)–(16) are the equations in respect of the wave-fixed reference frame that are corresponding to (1)–(4) and (11), respectively. To simplify usage of the symbols in the equations, the same alphabets as those in the laboratory reference frame are used in (12)–(16).

In order to solve for Equations (12)–(16), the boundary conditions are required at the cold (unreacted) and hot (reacted) ends. To a wave motion, the state before the wave is generally known. Therefore, the boundary conditions at the cold end are the Dirichlet type:

$$(u, \rho, p, T, E, Y)|_{x=-\infty} = (u_0, \rho_0, p_0, T_0, E_0, Y_0) \quad (17)$$

At $x = +\infty$, i.e. the hot end, the reaction is completed and therefore the state of the wave will recover the uniformity. Thus, Neumann boundary conditions should be imposed at the hot boundary:

$$\left(\frac{\partial u}{\partial x}, \frac{\partial \rho}{\partial x}, \frac{\partial p}{\partial x}, \frac{\partial T}{\partial x}, \frac{\partial E}{\partial x}, \frac{\partial Y}{\partial x} \right) \Big|_{x=+\infty} = (0, 0, 0, 0, 0, 0) \quad (18)$$

If all the terms on the right-hand side of the boundary conditions (17) are known, the problem (11)–(16) will be uniquely solved. But the velocity in (17), u_0 , is unknown, which is just the speed of the combustion wave propagation to be found. Therefore, we need additional conditions to make the problem solvable.

The additional conditions are imposed at the cold boundary, which are

$$\left(\frac{\partial u}{\partial x}, \frac{\partial \rho}{\partial x}, \frac{\partial p}{\partial x}, \frac{\partial T}{\partial x}, \frac{\partial E}{\partial x}, \frac{\partial Y}{\partial x} \right) \Big|_{x=-\infty} = (0, 0, 0, 0, 0, 0) \quad (19)$$

The boundary conditions (19) imply that the reaction rate is zero at the cold boundary. If the reaction rate at $x = -\infty$ were not zero that is termed cold boundary difficulty by (Williams, 1985), the combustible mixture, before the combustion wave turns up, would be burned out, because the cold boundary end is theoretically in the infinitely away place. Therefore, non-zero reaction rate at the cold end is clearly non-physical and boundary condition (19) is essential.

The problem (12)–(19) forms a general eigenvalue problem for steady and self-sustained premixed combustion wave propagations in which the speed of combustion wave, u_0 , is the eigenvalue of the problem to be found. There is always a trivial solution, zero solution, for the eigenvalue problem. Physically it represents that the combustion is self-extinguished after the ignition. In what follows, we are going to find the non-trivial solutions. The non-trivial solutions indicate the self-sustained combustion wave propagation modes. Mathematically they are called spectrum of the wave propagations.

3. Solutions

In order to solve the eigenvalue problem mentioned in Section 2, the analytical solutions of the problem are sought. After having the analytical solutions, an iterative algorithm for numerical computation of the combustion wave propagation and its speed is devised.

3.1. Integral solutions

Integrating the Equations (12)–(15) from $x = -\infty$ to $x = +\infty$ and also using the boundary condition (17)–(19), we can obtain

$$\rho_0 u_0 = \rho_b u_b \quad (20)$$

$$\rho_0 u_0^2 + p_0 = \rho_b u_b^2 + p_b \quad (21)$$

$$c_p T_0 + \frac{1}{2} u_0^2 + q_0 = c_p T_b + \frac{1}{2} u_b^2 \quad (22)$$

$$m \equiv \rho_0 u_0 = \rho_b u_b = - \int_{-\infty}^{+\infty} \rho \dot{\omega} dx \quad (23)$$

The subscript 0 and b denotes the quantities of the mixture at the cold and burned sides and c_p is the constant-pressure specific heat capacity and $q_0 = h_0 \cdot Y_0$ that is the total release heat in combustion and is constant when initial conditions are definite. The Equations (20)–(23) are an integration form of (12)–(15), in which u_0 or m is the eigenvalue. It should be noted that Equation (14) gives a direct relevance of the reaction courses that are controlled by the detailed chemical kinetics and the speed of combustion wave. It implies that distinct chemical kinetics would result in the different combustion wave propagation speed although the total release heat of combustion is same. This conclusion, however, is not accepted by some theories for fast combustion wave propagations, e.g. ZND (Zeldovich–von Neumann–Doering) detonation (Courant & Friedrichs, 1976; Döring, 1943; von Neumann, 1942; Williams, 1985; Zeldovich, 1940). At present, a steady and self-sustained detonation or ZND detonation is thought to theoretically have the minimal propagation speed within all the possible detonation modes, i.e. Chapman–Jouguet (C–J) detonation speed (Higgins, 2012), which is determined only by the total release heat in combustion and independent of the chemical kinetics. It should be pointed out that this theoretic detonation speed, in fact, has yet not been proved strictly and therefore is actually a conjecture.

In this work, it is further assumed that the gaseous mixtures involved in the course are the ideal gas and the thermal properties of the gas mixture such as specific heat capacity are constant and able to be calculated by the formulae of ideal gas, e.g. $c_p = R\gamma / \gamma - 1$, here R is the gas constant. Under the assumptions, we rewrite Equations (22)–(23) into Rayleigh line Equation (24) and Hugoniot Equation (25) (Williams, 1985):

$$M_0^2 \equiv \left(\frac{u_0}{a_0} \right)^2 = - \frac{\bar{p} - 1}{\gamma(\bar{p}^{-1} - 1)} \quad (24)$$

where $a = \sqrt{\gamma p / \rho}$ and M are the sonic speed and Mach number, respectively, and $\bar{p} = p_b / p_0$ and $\bar{\rho} = \rho_b / \rho_0$. Rayleigh line Equation (24) reflects the relationship between the flow velocity and the ratio of thermodynamic states before and behind the combustion wave.

$$\left(\bar{p} + \frac{\gamma - 1}{\gamma + 1} \right) \left(\bar{\rho}^{-1} - \frac{\gamma - 1}{\gamma + 1} \right) = \frac{4\gamma}{(\gamma + 1)^2} + 2\bar{q} \left(\frac{\gamma - 1}{\gamma + 1} \right) \quad (25)$$

where $\bar{q} = (\rho_0 / p_0) q_0$ is the normalised heat released by the reactions. Hugoniot Equation (25) indicates the relationship of the thermodynamic states ahead of and behind the combustion wave with the total release heat of combustion.

These two equations show that the state of the combustion wave at $x = +\infty$ is completely determined if the speed of combustion wave propagation (M_0) is known. Unfortunately, the speed of the combustion wave propagation is unknown to be found.

It is noted that the Equations (24) and (25) are only related to the total release heat of combustion but independent of the reaction processes controlled by the detailed chemical kinetics. In order to seek for the relationship between the speed of combustion wave propagation and the reaction rate or detailed chemical kinetics, we integrate (16) and obtain an algebraic Equation (26):

$$\begin{aligned} & \rho_b u_b \ln \left(\frac{p_b}{p_0} \right) - \rho_0 u_0 \ln \left(\frac{p_0}{p_0} \right) \\ &= -(\gamma - 1) \int_{-\infty}^{+\infty} \frac{\left[u \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial x} \right) + h_0^T \cdot \rho \dot{\omega} - \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} dx \end{aligned} \quad (26)$$

Not only does Equation (26) present the relationship between the speed of combustion wave propagation and chemical reaction rates or detailed chemical kinetics, but also give the effects of transport processes on the speed of combustion wave propagation. *It is an additional condition that allows the eigenvalue problems uniquely define the solution.*

Having Equation (26), we may define an averaged temperature of the combustion wave, T_a :

$$\frac{1}{T_a} \equiv -\frac{1}{m} \int_{-\infty}^{+\infty} \frac{\left[\frac{u}{q_0} \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial x} \right) + \frac{h_0^T \cdot \rho \dot{\omega}}{q_0} - \frac{1}{q_0} \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} dx \quad (27)$$

where $m = \rho_b u_b = \rho_u u_u$ which is just the eigenvalue to be found.

Further rewriting (16), we have

$$\frac{p_b/p_0}{\rho_b^\gamma/\rho_0^\gamma} = e^{(\gamma-1) \frac{q_0}{T_a}} \quad (28)$$

The above Equation can be rewritten in the form consistent with (24) and (25) as

$$\frac{\bar{p}}{\bar{\rho}^\gamma} = e^{(\gamma-1) \frac{q_0}{T_a}} \quad (29)$$

Using the Equations (24), (25) and (29), one can uniquely determine the speed of combustion wave propagation or eigenvalue of the problem (12)–(19). Therefore, these equations will be used for numerical computations of the combustion wave propagation speed in Section 3.4.

3.2. Formula for the speed of combustion wave propagation

The averaged temperature defined above expresses one important characteristic of the combustion wave propagation. From the equation (27), we see that it is directly related to the combustion wave propagation speed. Further analysis shows that the temperature satisfies the inequality (30), but the exact lower limit and upper limit of the averaged temperature are the averaged temperatures of the combustion waves at Chapman–Jouguet (C–J) deflagration and Chapman–Jouguet (C–J) detonation, respectively.

$$T_0 \leq T_a \leq T_b < T_0 + \frac{q_0}{c_p} \equiv T_0 + \frac{(\gamma - 1)}{\gamma} q_0 \quad (30)$$

Reformulating Equation (26), we will have an explicit expression of the eigenvalue or combustion wave propagation speed (31):

$$m \equiv (\gamma - 1) \left[\ln \left(\frac{\bar{\rho}^\gamma}{\bar{p}} \right) \right]^{-1} \int_{-\infty}^{+\infty} \frac{\left[u \frac{\partial}{\partial x} \left(\eta \frac{\partial u}{\partial x} \right) + h_0^T \cdot \rho \dot{\omega} - \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} dx \quad (31)$$

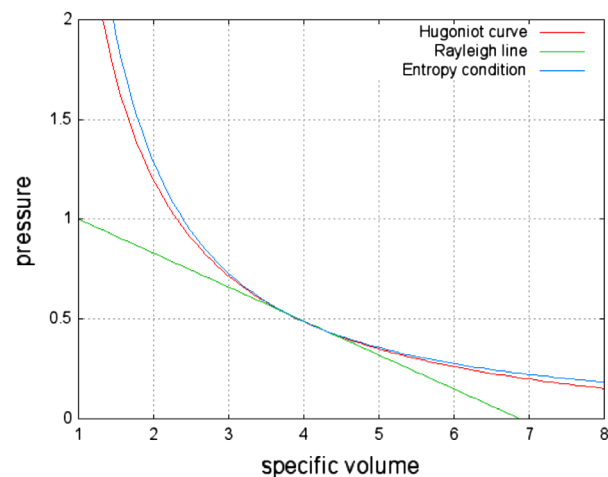
It is seen from (31) that the transport terms, the first and third terms in the integration, and the reaction rate, the second term in the integration, individually and independently contribute to the speed of the combustion wave propagation.

3.3. Selective mechanism of combustion wave

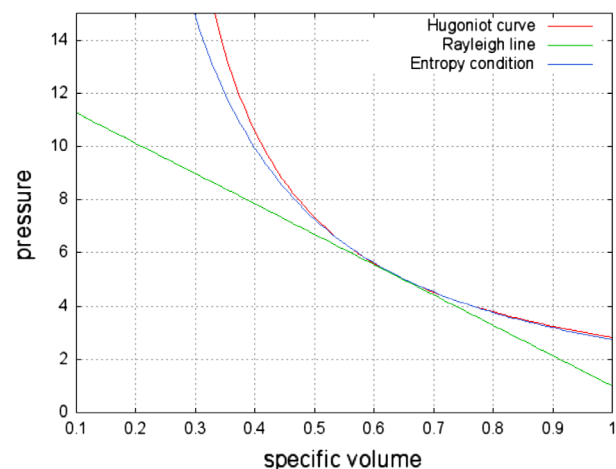
In order to intuitively represent the existence of a self-sustained combustion wave and understand the wave propagation, Figures 1 and 2 illustrate three Equations (24), (25) and (29) in the pressure-specific-volume plane for the four typical cases. The point crossed by the three curves shows the existence of the self-sustained combustion wave and the corresponding Rayleigh line gives the speed of combustion wave. A further explanation to the results will be given in Section 4.2.

The results in Figures 1 and 2 demonstrate an important mechanism—selective mechanism of combustion wave. The selective mechanism states when the total release heat of combustion is certain, the steady and self-sustained combustion wave could be a laminar flame with very slow propagation speed, or a fast deflagration, or detonation. To the laminar flame, the transport terms in (31), the first and third terms in the integration, play an major role to sustain the wave propagation, while the propagation of the fast deflagration and detonation is mainly maintained by the chemical reactions, i.e. the second term in the integration of (31), and such combustion wave concept, called spontaneous combustion wave, was introduced by (Zeldovich et al., 1985). Therefore,

Figure 1. C–J deflagration (a) and C–J detonation (b). They are the cross points of Hugoniot and Rayleigh line equations and entropy condition equation.

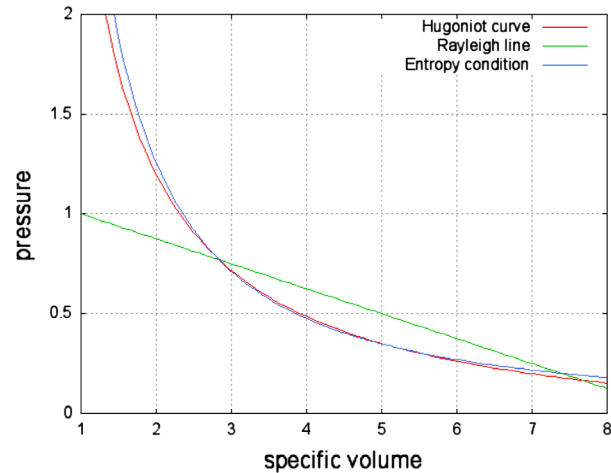


(a) C-J deflagration for $q_0 = 4.583$, $T_a = 1.4998$ and $M_u = 0.3485$

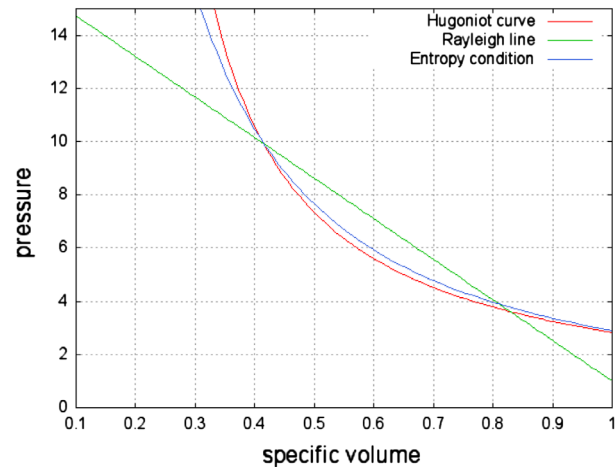


(b) C-J Detonation for $q_0 = 4.583$, $T_a = 1.8122$ and $M_u = 2.8536$

Figure 2. Two steady combustion waves: (a) deflagration and (b) detonation. They are neither C-J deflagration nor C-J detonation, but are at the cross points of Hugoniot and Rayleigh line equations and entropy condition equation.



(a) Deflagration for $q_0 = 4.583$, $T_a = 1.530$ and $M_u = 0.2988$



(b) Detonation for $q_0 = 4.583$, $T_a = 1.721$ and $M_u = 3.3004$

the theoretic model proposed in this work is actually a more complete theory for the spontaneous combustion waves.

In fact, the selective mechanism of combustion wave can be further interpreted using the principle of Rayleigh flow, heat addition flow (Hodge & Koenig, 1995). The principle states that a heat-addition flow can be uniquely defined if the total heat added and inlet flow state are known. Applying it to our eigenvalue problems, however, since the inlet flow velocity, i.e. speed of combustion wave propagation, is unknown, we need an additional condition for unique definition of the solution. The Equation (26) derived from this work provides the condition. Therefore, the Equation (26) can be called criterion for selection of combustion waves as well. Thus, the results in Figures 1 and 2 can be easily understood.

3.4. Numerical algorithms

Based on the analytical solutions above, numerical solutions for the problem (12)–(19) can be devised, which is summarised as follows. In the numerical solution, the Equations (12)–(15), or (20)–(22) and (15) are first solved through assuming a speed of combustion wave propagation as input

parameter. Then Equation (26) is employed to check the assumed speed. If the Equation is satisfied, the computation stops; otherwise redo the computational procedure after updating the assumed speed by the speed calculated from (26). The algorithm is written as

Numerical Algorithm

Step 0: Thermodynamic state ahead of the flame, ρ_0 , p_0 and T_0 , are known.

Step 1: Give a guess of the unburned mixture velocity, u_0^0 for starting the iteration.

Step 2: Integrate the Equations (12)–(15).

Step 3: A new unburned mixture velocity, u_0 , is solved from Equation (26).

Step 4: If $|u_0 - u_0^0| < \epsilon$, the calculation stops, otherwise update the unburned mixture velocity, u_0^0 and go to step 2. for iteration until the convergent criterion is met.

In the above algorithm, we see that (26) is used as the criterion to judge the convergence of the iterative solution and the scheme to update the wave speed in the previous iteration. This is one of the points that are different from the traditional methods. Since the criterion and update procedure are based on the exact formula of the eigenvalue (26), the computational iteration proposed above is more quickly converged to the solution.

Theoretically, the domain of the wave propagation is infinitely large. In the practical numerical calculation, however, the computational domain cannot be infinitely long and will be truncated to a finite domain which should include all the chemical reaction processes. In the implementation, when the rates of reactions at the two boundaries of the domain are less than 10^{-5} of the maximal reaction rate, the computational domain is deemed to include all the reactions. Out of the computational domain, the chemical reactions are almost zero and the physical quantities are therefore uniform, and therefore do not need to calculate them. In combustion theory, flame is defined as reaction zone (Williams, 1985). The length of the computational domain is also called flame thickness in the literature and the numerical computations are actually for the flame only.

The computational domain is meshed by 10^4 elements in this work. In the other words, the flame is resolved by 10^4 elements. The resolution is obviously fine enough. It should be noted that the length of the domain depends upon concrete chemical reactions and is unknown before the computation. Therefore, an adaptive method to select the length of the computational domain is employed, that is, the length of the domain is adjusted according to the prior-solution so that the domain includes all the reactions.

4. Results and discussions

In this section, an application of the proposed theoretical model is presented which will show the existence of the solutions of the eigenvalue problem introduced in Sections 2 and 3. For the sake of demonstration, only one species of reactants in the chemical reactions is involved in. Thus, the reaction Equation (4) is degenerated into the model same as the reaction progress equation describes. The works involving more complex reactions are in progress.

All the equations mentioned in the previous sections are nondimensionalised in the following computations. The sound speed, density, pressure and temperature at the cold boundary end, a_0 , ρ_0 , p_0 and T_0 , are used for the reference velocity, density, pressure and temperature, respectively. The reference length is the length of the computational domain or the flame thickness (see above texts).

It is assumed that the reaction rate is controlled by first-order Arrhenius kinetics that is written as

$$\dot{\omega} = -AYe^{-\frac{E_a}{T}} \quad (32)$$

The dimensionless pre-exponential factor can be expressed by $A = A' \cdot L/a_0$, here A' denotes the dimensional pre-exponential factor. The reference velocity is taken as the sound speed of the far field in this work and the reference length is determined according to the need of concrete application. The dimensionless activation energy is determined by $E_a = E'_a/(R \cdot T_0)$, in which E'_a and R are, respectively, the dimensional activation energy and gas constant. In the computations, the specific heat ratio is taken as $\gamma = 1.4$. The Reynolds number, Prandtl number and Schmidt number are, respectively, assumed to be 10^6 , 0.78 and 0.85.

The reader is reminded that since all the equations to be solved are dimensionless, the results presented below are all without units.

4.1. Numerical results

The numerical tests presented in this section are mainly for fast combustion waves. The purpose doing so is to demonstrate the existence of the fast combustion waves. Three groups of the waves are calculated using the method developed in Section 3. Each group has same release heat of combustion but distinct activation energy. The numerical results are presented in Table 1. The computations are very fast. Generally, numerical solutions can converge in the iterations of the order of 10.

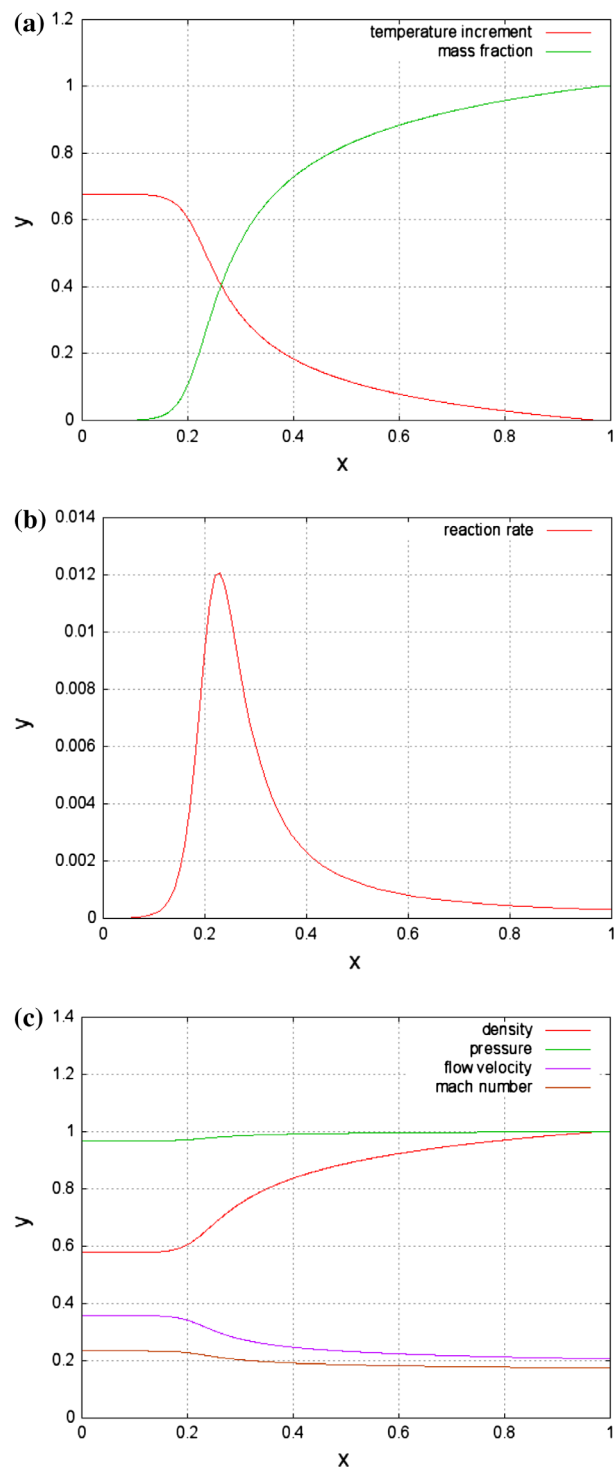
It is found that the modes of the combustion wave propagations are not continuous but discretely distributed between the conventional slow flame and Chapman–Jouguet deflagration. The calculated Mach number ahead of the flame, M_u , is defined by the ratio of the speed of the combustion wave propagation and local sonic speed. The calculated results show $M_u \approx 0.1 - 0.5$. These results are basically in agreement with the experimental results (Lee, 2001; Wu et al., 2007). From Table 1, one can see that the flame speed decreases and the averaged flame temperature increases with raising the activation energy.

Table 1. Modes of fast deflagrations in the three groups

| E_a | M_u | M_b | T_a |
|-----------------|--------|----------|----------|
| (a) $q_0 = 1.5$ | | | |
| 23 | 0.5155 | 1.0 | 1.169855 |
| 25 | 0.2428 | 0.298076 | 1.182689 |
| 30 | 0.2457 | 0.301823 | 1.177503 |
| 35 | 0.2420 | 0.297025 | 1.183932 |
| 40 | 0.2414 | 0.296237 | 1.185272 |
| 45 | 0.2150 | 0.262039 | 1.260602 |
| (b) $q_0 = 2.5$ | | | |
| 13 | 0.4391 | 1.0 | 1.250239 |
| 15 | 0.1747 | 0.233533 | 1.303065 |
| 20 | 0.1780 | 0.238263 | 1.294919 |
| 25 | 0.1734 | 0.297025 | 1.306243 |
| 30 | 0.1622 | 0.216087 | 1.344386 |
| 35 | 0.1367 | 0.181027 | 1.527641 |
| (c) $q_0 = 3.5$ | | | |
| 10 | 0.3873 | 1.0 | 1.364467 |
| 13 | 0.1389 | 0.200098 | 1.412425 |
| 18 | 0.1380 | 0.198593 | 1.415262 |
| 23 | 0.1328 | 0.190638 | 1.434328 |
| 28 | 0.1249 | 0.179160 | 1.474210 |
| 33 | 0.1059 | 0.151190 | 1.664397 |

Structure of a typical combustion wave is displayed in Figure 3 that is of $q_0 = 2.5$ and $E_a = 15$ (see Table 1). The x axis is normalised by the flame thickness. Figure 3(a) and (b) present profiles of the temperature increment with respect to the temperature ahead of the flame, mass fraction of reactant and reaction rate. One sees that there are three zones inside the flame, the temperature

Figure 3. Profiles of various physical quantities in the flame (x -axis is normalised by the flame thickness), (a) profiles of temperature increment with respect to the temperature ahead of the flame and mass fraction of reactant, (b) reaction rate and (c) profiles of density, pressure, velocity and Mach number.



development zone, main reaction zone and post reaction zone. Length of the temperature development zone depends upon the activation energy. The larger the activation energy, the longer the temperature development zone, vice versa. The main reaction zone is quite short, about 20% of the flame thickness, in which the change rate of the mass fraction is very sharp. The post reaction zone is a slow transition of the physical parameters to the burned region. To a small amount of activation energy, the structure of the combustion wave is similar to the structure of a laminar flame (Williams, 1985). But with an increase in the activation energy, the temperature development zone becomes longer, which shows that an longer induction zone is required. In the temperature development zone, the temperature rises in the exponent function until the reaction rate becomes significant large. This process can be explained by the thermal explosion theory (Zeldovich et al., 1985), which has been studied by many researchers, e.g. (Dold, 1989; Parkins, Blythe, & Crighton, 2000; Short & Dold, 1996).

The structure in Figure 3 (c) shows an increment in the flow velocity because of addition of the reaction heat. It is noted that the burned mixture flow velocity is equal to sum of the unburned mixture flow velocity and the increment in flow velocity because of addition of the heat of combustion. The larger the heat of combustion, the quicker the burned mixture flow velocity. One can also see that thermal expansion is generated inside the flame. In practical applications, the expansion drives the flame to move. Figure 3 (c) also shows a reduction of the pressure inside the flame.

where M_u and M_b are, respectively, Mach numbers of flame front and rear, and T_a is the averaged temperature defined by (27).

4.2. Discussions

Theoretically, two factors of the chemical reactions in combustion wave propagations influence the speeds of the wave propagations. One is the total release heat in combustions, i.e. heat of combustion. The other is the detailed chemical kinetics of chemical reactions. In what follows, we explore the details of the influencing and the relationships of the relevant parameters.

Hugoniot equation or curve (25) represents the relationship between the thermodynamic states of the mixture ahead of and behind the reaction zone, or flame. It is only related to the total release heat in combustions. When the total release heat in combustions is definite and the thermodynamic state of the mixture ahead of the reaction zone is certain, from Hugoniot Equation (25) we can see that the possible thermodynamic state of the mixture after the reaction zone is still of the infinitely possible states. This implies that the combustion wave propagation cannot be determined by the total release heat in combustions only.

On the other hand, Rayleigh line Equation (24) gives the relationship between the speed of combustion wave propagation and the thermodynamic state of the mixture after the reaction zone. Obviously, we cannot determine the speed of combustion wave propagation by (24) and (25), since Hugoniot Equation (25) cannot define the thermodynamic state of the mixture after the reaction zone as discussed above.

From (32), (3) and (14), we can see that the chemical kinetics directly controls the reaction rate and combustion-heat release rate. As a result, the chemical kinetics is certainly influencing the speed of combustion wave propagation. In this work, author developed a general relationship between the thermodynamic state of the mixture after the reaction zone and the combustion-heat release rate or chemical kinetics (26). Thus, when the chemical kinetics is given, we can determine the thermodynamic state of the mixture after the reaction zone through coupling solution of (25) and (26). Having the thermodynamic state of the mixture after the reaction zone, we can get the speed of combustion wave propagation using (24). All the three solutions (24), (25) and (26) are exact, and therefore this procedure for determining the speed of combustion wave propagation is very accurate. This is why the method proposed in this work is accurate and robust.

The algorithm in Section 3.4 is a numerical implementation of the above procedure. The steps 1 and 2 in the algorithm are for solving (25) and (24), while the step 3 is for solving (26).

5. Conclusion

In the wave-fix frame of reference, author of this paper presents a general model for steady and self-sustained combustion waves—the eigenvalue problem (12)–(19). The combustion wave can be either deflagration or detonation. Through analytically solving the eigenvalue problem, author found out an entropy condition (26) and mathematic formula for the speed of combustion wave propagations (31). From the formula, we can see the contribution of each component of the combustion processes to the speed of combustion wave propagation. The entropy condition associated with Hugoniot Equation and Rayleigh line equation shows that the mode of combustion wave propagation or distribution of spectrum of combustion waves is not continuous but discrete.

Furthermore, the analytical solutions found allow us to develop more effective algorithms and schemes for the numerical computations of the steady and self-sustained combustion wave propagation and its speed. An example of such algorithms is proposed in this work. Three groups of combustion wave propagations and their speeds are numerically calculated by the proposed algorithm. The numerical solutions converge very quickly. The numerical results show the detailed structures of the three groups of combustion waves and the correlation between their propagation speeds and chemical kinetics.

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Appendix A

Derivations of Entropy Condition and Averaged Flame Temperature in Laboratory Frame of Reference

The basic equations with respect to the laboratory frame of reference are unsteady and can be written as

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} = 0 \quad (\text{A1})$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} = \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) \quad (\text{A2})$$

$$\frac{\partial(\rho u E + u p)}{\partial x} = -h_0^T \cdot \rho \dot{\omega} + \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \cdot u \frac{\partial u}{\partial x} + \lambda \frac{\partial T}{\partial x} \right) \quad (\text{A3})$$

$$\frac{\partial(\rho Y)}{\partial t} + \frac{\partial(\rho u Y)}{\partial x} - \frac{\partial}{\partial x} \left(\rho D \frac{\partial Y}{\partial x} \right) = \rho \dot{\omega} \quad (\text{A4})$$

Through the transformation (A5), the Equations (A1)–(A3) can be reformulated as (A6)–(A8)

$$\frac{\partial \vec{v}}{\partial \vec{w}} = \left(\frac{\partial \vec{w}}{\partial \vec{v}} \right)^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ -\frac{u}{\rho} & \frac{1}{\rho} & 0 \\ \frac{(\gamma-1)u^2}{2} & -(\gamma-1)u & \gamma-1 \end{pmatrix} \quad (\text{A5})$$

where $\vec{w} = (\rho \quad \rho u \quad \rho E)^T$ and $\vec{v} = (\rho \quad u \quad p)^T$.

$$\frac{\partial \rho}{\partial t} + u \frac{\partial \rho}{\partial x} + \rho \frac{\partial(u)}{\partial x} = 0 \quad (\text{A6})$$

$$\frac{\partial(u)}{\partial t} + u \frac{\partial u}{\partial x} + \frac{1}{\rho} \frac{\partial(p)}{\partial x} = \frac{1}{\rho} \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) \quad (\text{A7})$$

$$\frac{\partial(p)}{\partial t} + \gamma p \frac{\partial u}{\partial x} + u \frac{\partial(p)}{\partial x} = (\gamma-1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right] \quad (\text{A8})$$

The system of Equations (A6)–(A8) is a hyperbolic system, and can be decomposed as

$$\begin{aligned} \frac{\partial \vec{v}}{\partial t} + \begin{pmatrix} u & \rho & 0 \\ 0 & u & \frac{1}{\rho} \\ 0 & \gamma p & u \end{pmatrix} \frac{\partial \vec{v}}{\partial x} &\equiv \frac{\partial \vec{v}}{\partial t} + A \frac{\partial \vec{v}}{\partial x} \\ &\equiv \frac{\partial \vec{v}}{\partial t} + L \Lambda L^{-1} \frac{\partial \vec{v}}{\partial x} = \begin{pmatrix} 0 & & \\ & \frac{1}{\rho} \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) & \\ & & (\gamma-1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right] \end{pmatrix} \end{aligned} \quad (\text{A9})$$

where Λ is a diagonal matrix and its three diagonal elements are the three eigenvalues written in (A10), which correspond to the speeds of the three waves (Courant & Friedrichs, 1976)

$$\vec{\lambda} = (u \quad u - a \quad u + a)^T \quad (\text{A10})$$

In Equation (A9), L is the Left characteristic matrix of A , which is defined as

$$L^{-1} = \begin{pmatrix} 1 & 0 & -\frac{1}{a^2} \\ 0 & \frac{1}{2} & -\frac{1}{2\rho a} \\ 0 & \frac{1}{2} & \frac{1}{2\rho a} \end{pmatrix}$$

The last two waves are the acoustic waves, and the first one is the entropic wave. This entropic wave is actually the combustion wave, or flame. It propagates at the local flow velocity. In order to solve for the flow velocity and the speed of flame, we transform the Equation (A9) to characteristic space through the inverse of the Left characteristic matrix, L , multiplying the two sides of Equation (A9)

$$\begin{aligned} L^{-1} \frac{\partial \vec{V}}{\partial t} + L^{-1} L \Lambda L^{-1} \frac{\partial \vec{V}}{\partial x} &\equiv \frac{\partial \vec{N}}{\partial t} + \Lambda \frac{\partial \vec{N}}{\partial x} \\ &= L^{-1} \begin{pmatrix} 0 \\ \frac{1}{\rho} \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) \\ (\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right] \end{pmatrix} \\ &= \begin{pmatrix} -(\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right] \\ \frac{1}{2} \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) - \frac{\sigma^2}{2a} \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right] \\ \frac{1}{2} \frac{\partial}{\partial x} \left(\frac{4}{3} \mu \frac{\partial u}{\partial x} \right) + \frac{(\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{2a} \end{pmatrix} \end{aligned} \quad (A11)$$

Where $d\vec{N} = \left(dp - \frac{dp}{a^2} du - \frac{dp}{\rho a} du + \frac{dp}{\rho a} \right)^T$. For the isentropic flow, e.g. the flows behind the flame, since the right-hand side terms of (A11) are zero, all the three components of $d\vec{N}$ are integrable, therefore, three Riemann invariants exist which is written as

$$(R_1 \quad R_2 \quad R_3)^T \equiv \left(\frac{p}{\rho} \quad u - \frac{2a}{\gamma - 1} \quad u + \frac{2a}{\gamma - 1} \right)^T \quad (A12)$$

As the terms on right-hand side of Equation (A11) inside the flame (see figure 1) are non-zero, not all the three Riemann invariants always exist. However, Riemann invariants for the first Equation of (A11) exists, because this equation involves only two variables and integrable. As a result, we have

$$\begin{aligned} \frac{\partial \ln R_1}{\partial t} + u \frac{\partial \ln R_1}{\partial x} &= -\gamma \frac{(\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{a^2} \\ &= -\frac{(\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} \end{aligned} \quad (A13)$$

where R_1 denotes the first Riemann invariant defined in (A12). Considering the continuity equation, the Equation (A13) is rewritten as the conservative form:

$$\frac{\partial (\rho \ln R_1)}{\partial t} + \frac{\partial (\rho u \ln R_1)}{\partial x} = -\frac{(\gamma - 1) \left[-\rho \dot{\omega} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right) \right]}{T} \quad (A14)$$

Now we back to the wave-fixed frame of reference. Since the flame propagates at constant speed, the Equation (A14) under the wave-fixed frame of reference becomes steady, but the flow velocity under the wave-fixed frame of reference will be obtained by that the original flow velocity subtracts

the flame speed. We use the same symbol to express it. Integrating the steady equation, we obtain an algebraic equation for the first Riemann invariant:

$$\begin{aligned} & \rho_b u_b \ln \left(\frac{p_b}{p'_b} \right) - \rho_u u_u \ln \left(\frac{p_u}{p'_u} \right) \\ &= -(\gamma - 1) \int_{-\infty}^{+\infty} \frac{[-\rho \dot{w} q_0 + \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right)]}{T} dx \end{aligned} \quad (\text{A15})$$

Now, we define the averaged flame temperature, T_a :

$$\frac{1}{T_a} \equiv -\frac{1}{m} \int_{-\infty}^{+\infty} \frac{[\rho \dot{w} q_0 - \frac{\partial}{\partial x} \left(\lambda \frac{\partial T}{\partial x} \right)]}{T} dx \quad (\text{A16})$$

where $m = \rho_b u_b = \rho_u u_u$. We ultimately obtain

$$\frac{p_b/p_u}{p'_b/p'_u} = e^{(\gamma-1) \frac{q_0}{T_a}} \quad (\text{A17})$$

Clearly, the averaged flame temperature satisfies

$$T_u \leq T_a \leq T_b < T_u + \frac{q_0}{c_p} \equiv T_u + \frac{(\gamma-1)}{\gamma} q_0 \quad (\text{A18})$$



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